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# Probabilistic Error Bounds for Reduced Order Modeling

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## ABSTRACT

Reduced order modeling has proven to be an effective tool when repeated execution of reactor analysis codes is required. ROM operates on the assumption that the intrinsic dimensionality of the associated reactor physics models is sufficiently small when compared to the nominal dimensionality of the input and output data streams. By employing a truncation technique with roots in linear algebra matrix decomposition theory, ROM effectively discards all components of the input and output data that have negligible impact on reactor attributes of interest. This manuscript introduces a mathematical approach to quantify the errors resulting from the discarded ROM components. As supported by numerical experiments, the introduced analysis proves that the contribution of the discarded components could be upper-bounded with an overwhelmingly high probability. The reverse of this statement implies that the ROM algorithm can self-adapt to determine the level of the reduction needed such that the maximum resulting reduction error is below a given tolerance limit that is set by the user.

**Key Words:** Reduced order modeling, Error bounds

## 1 INTRODUCTION

Recently, there has been an increased interest in reduced order modeling algorithms for reactor physics simulation. This is primarily driven by the best-estimates plus uncertainty (BEPU) approach, first championed by the industry until its adoption into law by the US-NRC in 1988. To fully realize the benefits of the BEPU approach, the uncertainties of the simulation predictions must be properly characterized. Uncertainty characterization (UC) implies the capabilities to identify, quantify, and prioritize the various sources of uncertainties. These three capabilities require repeated model executions which proves to be an increasingly taxing endeavor, especially with the continuous increase in the modeling details sought to improve fidelity.

Reduced order modeling is premised on the observation that the true dimensionality of reactor physics simulation codes is rather small, implying that the associated uncertainty sources that affect model behavior must also be rather small notwithstanding their nominal number is very large. With a small number of uncertainty sources, uncertainty characterization becomes a computationally tractable practice. This follows because the computational cost of performing UC depends on the number of uncertainty sources, which absent reduction could number in the millions for typical reactor physics simulation.

## 2 ROM ERROR BOUND CONSTRUCTION

To describe the contribution of this manuscript, basic definition of ROM is first introduced. Consider a model of reactor physics simulation of the form:

$$y = f(x) \tag{1}$$

where $x \in \mathbb{R}^n$ are reactor physics parameters, e.g., cross-sections, $y \in \mathbb{R}^m$ are reactor responses of interest e.g., eigenvalue, peak clad temperature, etc., and $n$ and $m$ are the numbers of parameters and responses, respectively. The simulation, represented by the function $f$, is assumed to be a black box. The goal of any ROM approach is replace the original simulation with an approximate representation $\tilde{f}$ that can be used in lieu of the original simulation for computationally intensive analyses such as UC. To ensure reliability of the ROM approximation $\tilde{f}$, the following criterion must be satisfied:

$$\left\| f(x) - \tilde{f}(x) \right\| \leq \varepsilon \text{ for all } x \in S \tag{2}$$

where $\varepsilon$ is a to-be-determined upper-bound, and $S$ defines the region of applicability. If such upper-bound exists, one can adjust the level of reduction to ensure that the bound matches the confidence one has in the original simulation predictions. In such case, both $f$ and $\tilde{f}$ would provide the same level of confidence for any subsequent analysis.

In our analysis, the ROM approximation $\tilde{f}$ has the general form:

$$\tilde{f}(x) = \mathbf{N} f(\mathbf{K}x)$$

where both **N** and **K** are rank-deficient matrix operators such that:

$$\mathbf{N} \in \mathbb{R}^{m\times m},\ \dim\left(\mathrm{R}(\mathbf{N})\right) = r_m, \text{ and } r_m \ll \min(m,n),$$

$$\mathbf{K} \in \mathbb{R}^{n\times n},\ \dim\left(\mathrm{R}(\mathbf{K})\right) = r_n, \text{ and } r_n \ll \min(m,n).$$

These matrices identify active subspaces in the space of input parameters and output responses. The implication is that few degrees of freedom in the input space are needed to capture all possible model variations, and the output responses have only a small number of degrees of freedom as well, implying large degrees of correlation exist therein. This knowledge allows one to craft uncertainty quantification and sensitivity analysis techniques in such a manner that reduces the required number of forward and/or adjoint model executions necessary to complete the respective analyses. See earlier work for more details on these approaches [1, 2].

In practice, the error operator is inaccessible but can be sampled and aggregated in a matrix **E** whose $ij^{th}$ element represents the error in the $i^{th}$ response of the $j^{th}$ sample, written as:

$$[\mathbf{E}]_{ij} = \frac{f_i(x_j) - \mathbf{Q}_y(i,:)\mathbf{Q}_y^T(i,:)\, f_i(\mathbf{Q}_x\mathbf{Q}_x^T x_j)}{f_i(x_j)} \tag{3}$$

The matrix **E** calculates the discarded component of function *f*. Each row of **E** represents a response, implying that if one treats each row as a matrix, it is possible to calculate a different error bound for each response. This allows one to compute the individual responses' errors since each response is expected to have its own reduction error. To achieve that: consider a matrix $\mathbf{E} \in \mathbb{R}^{m\times N}$ and a random vector $w \in \mathbb{R}^{N}$ where $N$ is the number of sampled responses such that $\mathrm{w}_i \sim \mathcal{D}$, where $\mathcal{D}$ is binomial distribution with a probability of success of 0.9. Then *w* can be used to estimate the largest and smallest eigenvalue and hence the 2-norm of **E** via:

$$\mathbb{P}\left\{\left\|\mathbf{E}\right\| \le \eta \max_{i=1,2,\cdots s}\left\|\mathbf{E}w^{(i)}\right\|\right\} \ge 1-\left(\int_0^{\frac{1}{\eta^2}} pdf_{w_1^2}\left(t\right)dt\right)^s, \tag{4}$$

where the multiplier $\eta \ge 1/\left\|w\right\|$ is numerically evaluated to be 1.0164 for binomial distribution and for a success probability of 0.9. For more details about this approach and the proof of Eq. (4), the reader may consult the following references [3, 4, 5, 6].

The main goal of this paper is to show that one can satisfy Eq. (4) for any given **N** and **K** matrices with an overwhelmingly high probability. Computing an error bound for general reduction operators is important because in general multi-physics models, one may obtain a reduction operator using a lower-fidelity model when the high fidelity model is too expensive to execute in search of the ROM active subspace. Another situation occurs when the input for a given physics model is produced by another physics model. In such case, one could use the forward model executions of the upstream physics model to calculate an active subspace for the downstream physics. Therefore, it is important to capture the reduction errors for general matrix reduction operators.

If the distribution of *w* and the multiplier $\eta$ are selected such that the integral on the right hand side is 0.1, the probability that the estimated bound is larger than the 2-norm of the error is given by: $p = 1-10^{-s}$, where *s* is a small integer that corresponds to an additional number of matrix-vector multiplications. Typically, we employ a value of *s* equal to 10 to ensure extremely high probability. In support of verifying the proposed algorithm however, this manuscript will employ *s*=1 to give rise to situations when the estimated error bound fails to bound the actual errors with probability of 10%. Multiple numerical experiments will be devised to test the upper-bound and the probability of failure as predicted by the theory.

## 3 NUMERICAL EXPERIMENTS AND RESULTS

This section will employ a number of experiments to demonstrate the ability to calculate an upper-bound on the reduction error. The first experiment will focus on a direct ROM application to identify the active subspace and calculate the associated reduction error and probability of failure. The second experiment will employ the reduction operators determined using a given set of conditions (low burnup, hot full power) to test its adequacy for other conditions (higher burnup and cold conditions). This capability will prove useful in model validation activities relying on the use of the proposed reduction techniques, where now one must determine whether the developed reduced model will be adequate for a wide range of operating conditions.

### 3.1 Case Study 1:

This case study employs a pin cell depleted to (3.0 GWd/MTU) as the reference model used to identify the active subspaces for the parameters and the responses spaces. SCALE 6.1 is used for the computational purposes, sequences like t-depl, t-newt, tsunami-2d and SAMS 5.0 are needed for the depletion, neutronics calculations and sensitivity analysis respectively [7]. The original parameter space contains 7 nuclides * 2 reactions * 238 energy groups=3332 parameters, whereas the nominal dimension for the response space is 238 representing material flux at 238 energy groups. For illustration, a very small rank is assumed to ensure that the actual errors are large enough to possibly fail the theoretical error bound proposed here. In all the tests, a value of $s=1$ is employed to maximize the number of failures for the sake of demonstration. In the series of figures below, the actual probability of failure is indicated on the top of the left graphs.

Figs. 1 through 4 display the results of the first case study. The same responses are employed for both case studies. In the odd-numbered figures, the response is the total collision rate in the energy range 1.85 to 2.35 MeV. The even figures show the same response but in the thermal range between 0.975 and 1.0 eV. We use these small ranges to depict the power of the reduction in capturing localized responses. In each of the figures, the left graph compares the actual error resulting from the reduction to the error bound calculated from Eq. (4). The 45-degree solid line indicates the limit of the failure region, i.e., when the actual error exceeds the bound predicted by the theory. The right graphs show the actual variation of the response due to a random perturbation of 30% in the parameters.

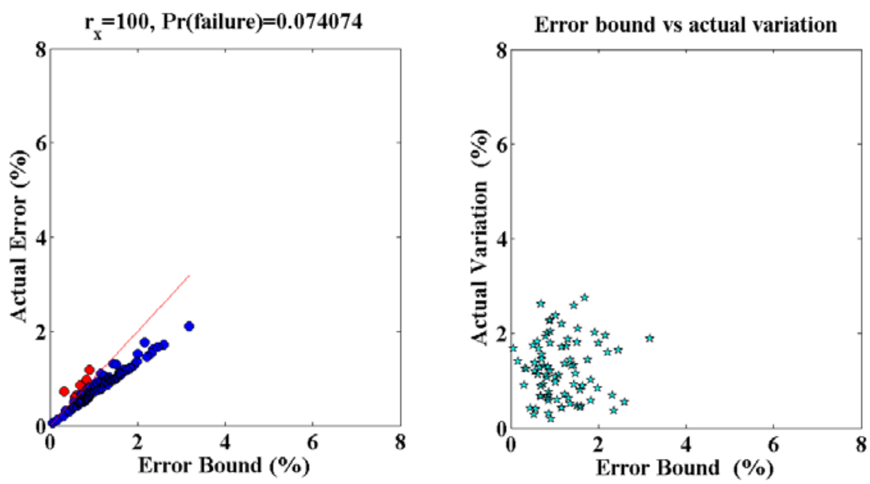


**Figure 1. Fast Collision Rate Errors – Parameter Reduction Only**

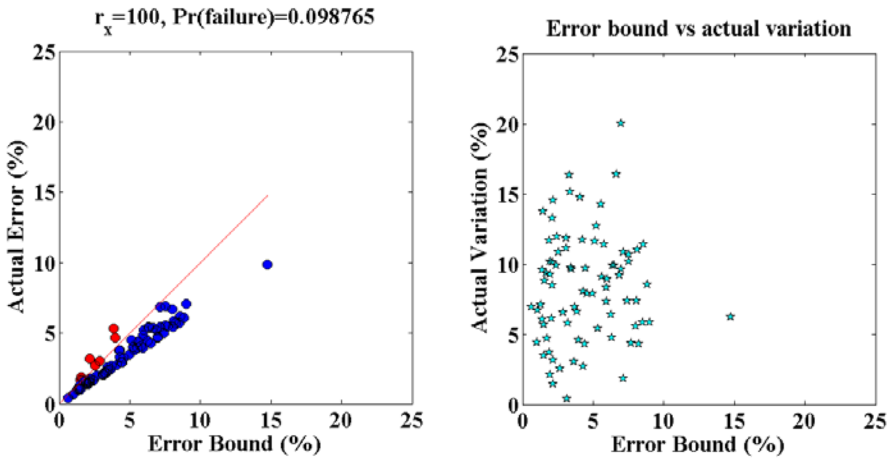


**Figure 2. Thermal Collision Rate Errors – Parameter Reduction Only**

Figs. 1 and 2 show a parameter-only-based reduction, meaning that the reduction is rendered at the parameter space. Both the level of reduction in terms of the rank of the active parameter subspace $r_x$, and the actual probability of failure are shown on the top of the right graph. Reader should remember that we picked $s$ and the multiplier in equation (4) such that the probability of success is 0.9. In reality $s$ is picked to be 5 which results in a probability of success of 99.999%. Figs. 3 and 4 employ response-based reduction only, implying no reduction in the parameter space. The rank of response active subspace $r_y$ is indicated in a similar manner.

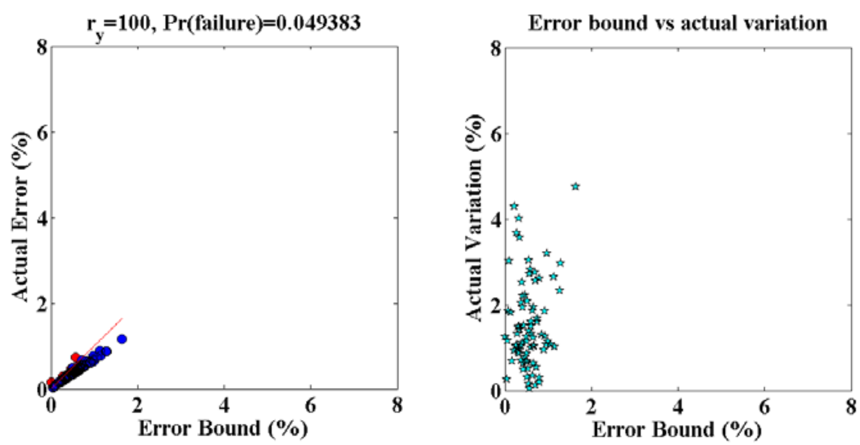


**Figure 3. Fast Collision Rate Errors – Response Reduction Only**

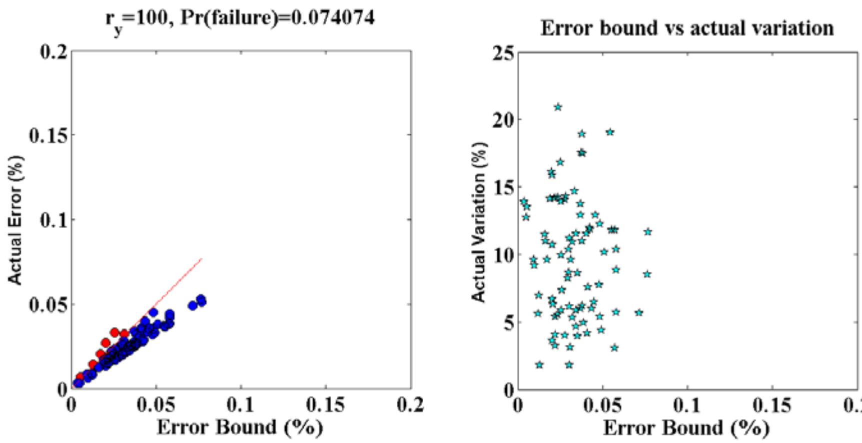


**Figure 4. Thermal Collision Rate Errors – Response Reduction Only**

Notice that the reduction errors calculated will depend on whether the parameter-based reduction captures the important parameter directions that control the model response variations. Moreover, the response reduction, if not captured correctly, will miss directions along which the response is expected to vary. This situation will be clearer when we consider different physics conditions as done in the next case study.

### 3.2 Case Study 2:

This case study employs the active subspaces extracted from the previous reference model to predict the response variations at different physics conditions. We employ a 24 GWd/MTU depleted fuel simulated at cold conditions. This emulates the effect of starting up a reactor with a once-burned fuel.

Figs. 5 through 8 correspond respectively to Figs. 1 through 4, where now the model is being evaluated at different physics conditions, using the reduction results from the previous case study, i.e., same ranks for parameter and response spaces, same responses, and same size of parameter perturbations. The idea here is to check whether the model reduced at hot conditions could be employed at sufficiently different physics conditions.

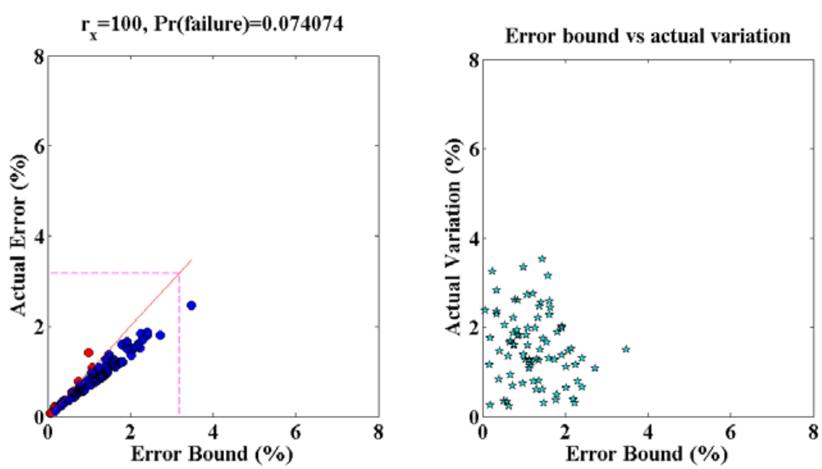


**Figure 5. Fast Collision Rate Errors - Parameter Reduction Only**

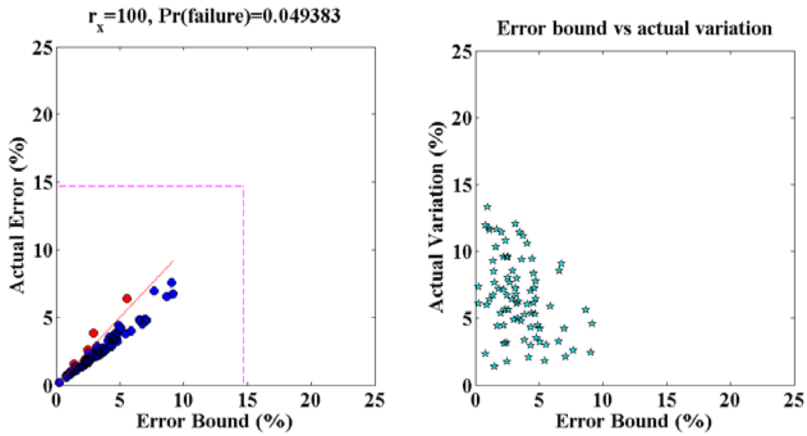


**Figure 6. Thermal Collision Rate Errors - Parameter Reduction Only**

Figs. 5 and 6 show that the actual errors and the predicted bounds due to the parameter reduction are slightly higher than the errors in figs. 1 and 2. This indicates that the active subspace extracted using the reference model have approximately the same level of accuracy at new physics conditions.

Figs. 7 and 8 behave in a different fashion, where now results indicate that the actual errors and their bounds have noticeably increased beyond those in Figs. 3 and 4. This indicates that the responses at the new physics conditions are changing along new directions in the response space that are not captured by the reference physics models. Also, notice that in all cases, the actual probability of failure is always less than the theoretical value of $1\text{-}10^{-s}$. Smaller number of failures were observed in Figs. 7 and 8; the reason for this remains to be investigated. We recall here that the failure probability is chosen to be 10% which is extremely high. In reality, the failure probability is set to be extremely small to ensure that its dependence on core conditions is negligible.

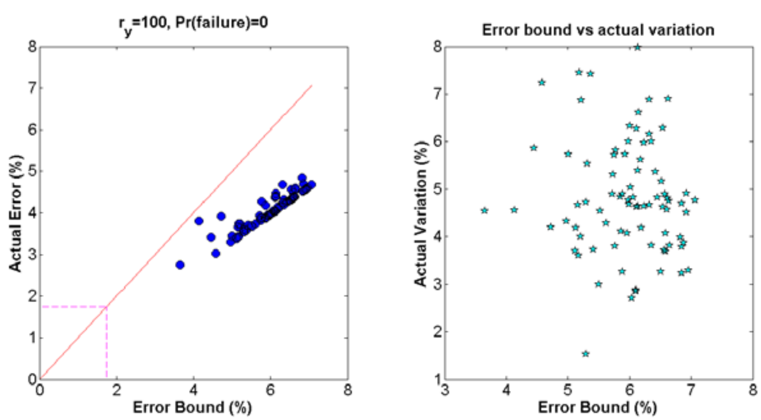


**Figure 7. Fast Collision Rate Errors - Response Reduction Only**

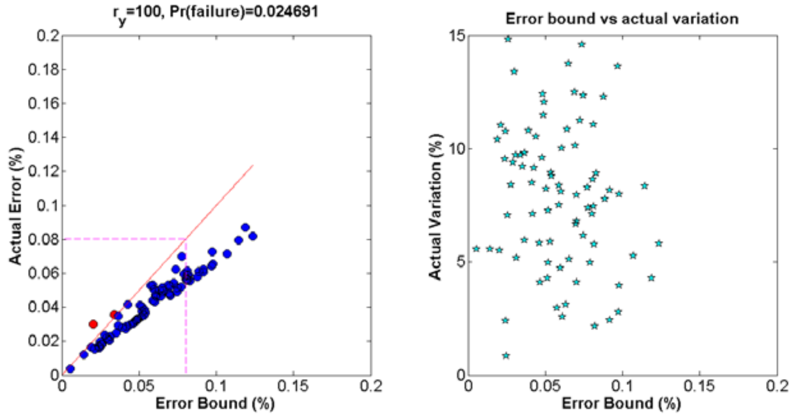


**Figure 8. Thermal Collision Rate Errors - Response Reduction Only**

## 4 CONCLUSIONS:

This manuscript has investigated the ability of ROM techniques to upper-bound the error resulting from the reduction. This is an important characteristic for any ROM to ensure reliability of the reduced model for subsequent engineering analyses, such as uncertainty and sensitivity analysis. More importantly, this summary has shown a practical way by which the ROM errors can be evaluated for general reduction operators. This is invaluable when dealing with high fidelity codes that can only be executed few times, and it is difficult to extract their active subspaces. Another important application of this work is the reduction of multi-physics models, where the active subspace generated by one physics model is used as the basis for reducing the input space for another physics model.

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